

Reduction and Unfolding for Quantum Systems: the Hydrogen Atom

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Abstract

In this paper we propose a “quantum reduction procedure” based on the reduction of algebras of differential operators on a manifold. We use these techniques to show, in a systematic way, how to relate the hydrogen atom to a family of quantum harmonic oscillators, by the means of the Kustaaheimo-Stiefel fibration.

1 Introduction

Reduction procedures have been extensively studied in the classical setting, dealing mainly with Hamiltonian dynamics ([1], [2], [3]) but also Lagrangian dynamics or more general ones ([4],[5], [6]). It has been noted that different classes of completely integrable systems arise as reduction of free (or simpler) ones in higher dimensions ([7]): this has been the motivation for the development of unfolding techniques, i.e. the converse of reduction, a still open field. In this context some of us (A.D., G.M.) have studied in a systematic way how to relate the Kepler problem to a family of harmonic oscillators ([8]); the aim of the present paper is to exploit this same relationship in the quantum setting, focusing on a possible method of quantum reduction that we propose here and on a possible way to tackle the unfolding procedure.

The problem we consider as a case of study has been widely studied and the above relationship has been established using many different approaches ([9],[10], [11],[12],[13],[14],[15]); so, the results are well known ([16], [17]). However, all these approaches lack of a systematic procedure underlying the computational results: moved by this, in this paper we try to insert the problem related to the hydrogen atom in a more general framework, i.e. that of “quantum reduction”. Although the problem of reduction has been given

a lot of consideration in the classical setting, the same has not happened in a systematic way in the quantum setting. An attempt toward this direction has been done by Perelomov and Olshanetsky in [19]. This article provides examples and motivations to the idea that it could be useful to develop an unfolding procedure also in the quantum setting. Some other proposals are given in [20], [21], and also [22]. Within this context, the present paper tries to clarify some methodological aspects of these procedures, that are nevertheless not yet well systematized, and to make a further step towards the development of a “quantum” reduction.

Our proposal has its starting point in the analysis of the classical reduction procedure, which, in an algebraic language ([6]), can be seen as a homomorphism between selected Lie algebras of vector fields on manifolds, associated with a suitable map between the configuration manifolds. In the same spirit, we propose a “quantum reduction” procedure based on a homomorphism between Lie algebras of differential operators (of arbitrary degree) on manifolds. Our choice to deal with differential operators built on the “configuration space” has been made to emphasize the geometrical aspects of a quantum mechanical system, and to work in strict analogy with the classical case. Nevertheless, we treat the problem as a purely quantum one, without resorting to any kind of quantization.

For the sake of clarity, we decompose the problem in two steps. The first one is the development of a reduction procedure for differential operators on a manifold \mathcal{M} , i.e. acting on the functions on \mathcal{M} , without dealing with the Hilbert space structure, that will be considered in the second step. The first step could be thought of as the reduction of a partial differential equation on a manifold to one on a manifold of lower dimensions. The definitions and results we propose are therefore not necessarily linked to quantum mechanics, since they concern only differential equations, so they can be used in several physical contexts.

However, since we are interested in quantum mechanics, the Hilbert space structure plays a relevant role and has to be taken into account. However, there is not an algorithmic way to build the relationship between Hilbert spaces: it strongly depends on the features of the map between the configuration manifolds, and this has to be analyzed case by case.

All this has been worked explicitly in the case of the hydrogen atom, where we have been able to restrict the arbitrariness in the choice of the unfolding operator, by means of an “educated guess” motivated by symmetry considerations. Our procedure emphasizes the relationship of the hydrogen atom with a one-parameter *family* of harmonic oscillators.

Motivated by what happens in our case of study, we conclude with an attempt toward the analysis of the possible role of reparametrization in the quantum setting. As far as we know, this topic has never been fully exploited: in our opinion, this would shed more light on the relationship between classical and quantum settings, both physically and mathematically.

The paper is organized as follows.

In section 2, after recalling a way to deal with differential operators (of any degree) on a manifold, we introduce and motivate the definition of “projectable differential operator”. In the ending subsection we give some additional details about the projectability of differential operators on $\mathbb{R}^4 - \{0\} \equiv \mathbb{R}_0^4$ on differential operators on $\mathbb{R}^3 - \{0\} \equiv \mathbb{R}_0^3$ with respect to the so-called Kustaanheimo-Stiefel map.

In section 3 we apply these techniques to the hydrogen atom, introducing a possible “quantum reduction procedure”. Our approach naturally provides the relation with a one parameter family of harmonic oscillators, as in the classical case. Moreover, we are able to recover usual results about the eigenvalue problem and the algebra of symmetry (section 3.1 and 3.2 respectively).

In the last section, we comments upon the role of the “reparametrization”, which was an important feature of the classical case, also in the quantum setting.

2 Differential operators

The aim of this section is to give a short review to recall how to deal with differential operators on a manifold. In the following we will restrict our attention to finite dimensional Hausdorff, locally compact C^∞ -manifolds.

We will start by introducing differential operators in \mathbb{R}^n , giving an algebraic characterization that will make us able to deal with differential operators on an arbitrary manifold (for a mathematical treatment of the topic see [23]). Let us consider the algebra $\mathcal{A} = C^\infty(\mathbb{R}^n)$ of infinitely differentiable functions on \mathbb{R}^n : in standard textbooks (e.g. [24]) a *differential operator of degree at most k* is defined as a linear map $D^k : \mathcal{A} \rightarrow \mathcal{A}$ of the form:

$$D^k = \sum_{|\sigma| \leq k} g_\sigma \frac{\partial^{|\sigma|}}{\partial x_\sigma} \quad g_\sigma \in \mathcal{A} \quad (2.1)$$

where $\sigma = (i_1, \dots, i_n)$, $|\sigma| = i_1 + i_2 + \dots + i_n$ and

$$\frac{\partial^{|\sigma|}}{\partial x_\sigma} = \frac{\partial^{|\sigma|}}{\partial x_1^{i_1} \dots \partial x_n^{i_n}} \quad (2.2)$$

This is a standard definition; however, one can give an algebraic characterization suitable for a generalization to arbitrary smooth manifolds. One can start considering the following commutator relation

$$\left[\frac{\partial}{\partial x_i}, \hat{f} \right] = \frac{\partial f}{\partial x_i} \quad (2.3)$$

where \hat{f} is understood to be the multiplicative operator $\hat{f} : g \rightarrow fg$, with $f, g \in \mathcal{A}$; then one can verify that

$$\left[\frac{\partial^{|\sigma|}}{\partial x_\sigma}, \hat{f} \right] = \sum_{\tau+\nu=\sigma} c_\tau \frac{\partial^{|\tau|} f}{\partial x_\tau} \frac{\partial^{|\nu|}}{\partial x_\nu} \quad (2.4)$$

with $|\tau| > 0$ and c_τ constants. From this it easily follows that

$$[D^k, \hat{f}] = \sum_{|\sigma| \leq k} g_\sigma \left[\frac{\partial^{|\sigma|}}{\partial x_\sigma}, \hat{f} \right] \quad (2.5)$$

is a differential operator of degree at most $k-1$. Iterating for a set of $k+1$ functions $f_0, f_1, \dots, f_k \in \mathcal{A}$, one finds that

$$[[\dots [D^k, \hat{f}_0], \hat{f}_1], \dots, \hat{f}_k] = 0 \quad (2.6)$$

The important fact is that it is possible to prove the converse, namely that a linear operator satisfying the property above for each set of $k+1$ elements in \mathcal{A} is necessarily of the form (2.1).

Using this algebraic characterization, one can generalize the notion of differential operator to an arbitrary manifold without referring to coordinates, by using its algebra of smooth functions. That is, one takes equation (2.6) as the definition of a differential operator with degree equal to the least number of elements of the algebra satisfying this equation minus 1.

In particular, differential operators of degree 1 which annihilate constant functions within the algebra \mathcal{A} (the constants) are derivations of \mathcal{A} , since it follows from equation 2.6 that they satisfy Leibniz rule with respect to the Abelian product in \mathcal{A} . It is well known that derivations on the algebra of functions on a manifold are vector fields on that manifold.

Moreover, one can deal with differential operators on a manifold \mathcal{M} as the elements of the enveloping algebra of the (infinite dimensional) Lie algebra of vector fields on \mathcal{M} , with the associative product obtained from the “composition” of derivations, and functions over \mathcal{M} .

The set of all the differential operators of any degree on \mathcal{M} , which we denote $\mathcal{D}(\mathcal{M})$, can be given a structure of a graded algebra, and also of a module over the algebra $\mathcal{F}(\mathcal{M})$ (see e.g. [24]). If the manifold is parallelizable, i.e. if the cross sections of the tangent bundle are a free module on \mathcal{A} , one has that the differential operators are a free module on \mathcal{A} , with a basis given by monomials in a finite number of vector fields and the identity function. If the manifold is not parallelizable we have projective modules. The case of free modules is simpler and we shall make some general statements in such a framework. Before doing that, let us now clarify the notion of projectability of a differential operator of an arbitrary degree, which will be at the core of our following analysis.

The preliminary ingredients are two manifolds \mathcal{M} and \mathcal{N} , and a submersion¹ $\pi : \mathcal{M} \rightarrow \mathcal{N}$. The starting point is the well known ([30], [3]) definition of projectability of a vector field on \mathcal{M} onto a vector field on \mathcal{N} , i.e. $\mathbf{X} \in \chi(\mathcal{M})$ is projectable with projection $\tilde{\mathbf{X}} \in \chi(\mathcal{N})$ if

$$\begin{array}{ccc} T\mathcal{M} & \xrightarrow{T\pi} & T\mathcal{N} \\ \mathbf{x} \uparrow & & \uparrow \tilde{\mathbf{x}} \\ \mathcal{M} & \xrightarrow{\pi} & \mathcal{N} \end{array} \quad (2.7)$$

Following the previous line, one can recast this definition in purely algebraic terms, which is more suitable for a generalization. At this aim, we will use the fact that an arbitrary manifold \mathcal{M} is perfectly encoded in its algebra of smooth functions $\mathcal{F}(\mathcal{M}) = C^\infty(\mathcal{M})$. In this context, one knows by general results that the submersion $\pi : \mathcal{M} \rightarrow \mathcal{N}$ gives rise to an injective homomorphism $\pi^* : \mathcal{F}(\mathcal{N}) \rightarrow \mathcal{F}(\mathcal{M})$, that allows one to consider $\mathcal{F}(\mathcal{N})$ as a subalgebra of $\mathcal{F}(\mathcal{M})$.

Since a vector field on a manifold is a derivation of its algebra of functions, one can prove ([3]) that the above definition 2.7 of projectability is equivalent to require that

$$\mathbf{X}(\mathcal{F}(\mathcal{N})) \subset \mathcal{F}(\mathcal{N}) \quad (2.8)$$

In other words \mathbf{X} is projectable if the subalgebra $\mathcal{F}(\mathcal{N})$ is invariant under the action of \mathbf{X} as a derivation. When \mathbf{X} is projectable, its projection is $\tilde{\mathbf{X}} = \mathbf{X}|_{\mathcal{F}(\mathcal{N})}$, i.e. the restriction of \mathbf{X} to $\mathcal{F}(\mathcal{N})$ as a linear operator.

These considerations lead us naturally to an extension of the definition of projectability for a differential² operator of arbitrary degree, in that a differential operator D^k of degree at most k will be called projectable (with respect to π) iff

$$D^k(\mathcal{F}(\mathcal{N})) \subset \mathcal{F}(\mathcal{N}) \quad (2.9)$$

As above, the projection of D^k will be $\tilde{D}^k = D^k|_{\mathcal{F}(\mathcal{N})}$.

Remark: The projectable differential operators (with respect to a given map) are a subalgebra of the whole graded algebra of differential operators on a given manifold; in fact, it is easy to show that they are closed under the operations of addition and composition of linear maps. Anyhow, they cannot be given a structure of submodule of the module $\mathcal{D}(\mathcal{M})$ over the algebra $\mathcal{F}(\mathcal{M})$, but only of a module over the algebra $\mathcal{F}(\mathcal{N})$.

2.1 Differential operators and the KS fibration

We are now going to give few additional details about the mathematical setting of our case of study, underlining its main characteristic features in

¹Obviously this requires $m = \dim \mathcal{M} > n = \dim \mathcal{N}$.

²Actually the definition we suggest is valid for a general linear operator, since it involves only the linear structure of the subalgebra

relationship with the above setting.

In this section we will deal only with differential operators on $\mathcal{F}(\mathcal{M})$, not considering the additional structures (e.g. the Hilbert space structure) that nevertheless are necessary for quantum mechanics; we postpone such consideration to a later section, pointing out that the following results are valid in the more general setting of the reduction of arbitrary differential equations. In the case at hand, we will consider the problem of the projectability of differential operators on $\mathbb{R}^4 - \{0\} \equiv \mathbb{R}_0^4$ on differential operators on $\mathbb{R}^3 - \{0\} \equiv \mathbb{R}_0^3$ with respect to the so-called Kustaanheimo-Stiefel map. In particular, we will consider in greater detail second order differential operators, since the ones we are interested in are of this form. For this purpose, let us recall some features of this map, first introduced in [28].

The main idea behind the construction of this map relies on the observation that \mathbb{R}_0^3 and \mathbb{R}_0^4 may be given a structure of trivial bundles over spheres, i.e. $\mathbb{R}_0^3 = S^2 \times \mathbb{R}^+$ and $\mathbb{R}_0^4 = S^3 \times \mathbb{R}^+$. Then one starts from the well know Hopf map $\pi_H : S^3 \rightarrow S^2$ ([26]); identifying S^3 with $SU(2)$, π_H may be represented as ([27])

$$\pi_H : s \in SU(2) \rightarrow \vec{x} \in S^2 : s\sigma_3s^{-1} = x^i\sigma_i \quad (2.10)$$

where σ_i are the Pauli matrices and x^i are cartesian coordinates in \mathbb{R}_0^3 . Now one may (not uniquely) extend the Hopf map to $\mathbb{R}_0^4 \rightarrow \mathbb{R}_0^3$ by introducing polar coordinates in $S^3 \times \mathbb{R}^+$; setting

$$g = Rs \quad \text{with} \quad s \in SU(2), R \in \mathbb{R}^+ \quad (2.11)$$

we may define

$$\pi_{KS} : g \in \mathbb{R}_0^4 \rightarrow \vec{x} \in \mathbb{R}_0^3 : x^k\sigma_k = g\sigma_3g^\dagger = R^2s\sigma_3s^{-1} \quad (2.12)$$

In a cartesian system of coordinates one has explicitly

$$\begin{aligned} x_1 &= 2(y_1y_3 + y_2y_0) \\ x_2 &= 2(y_2y_3 - y_1y_0) \\ x_3 &= y_1^2 + y_2^2 - y_3^2 - y_0^2 \end{aligned} \quad (2.13)$$

Moreover one finds that

$$\sqrt{x^i x_i} = r = R^2 = y^i y_i \quad (2.14)$$

It is important to notice that the map π_{KS} above constructed, which in the following we refer to as KS-fibration, defines a principal fibration $\mathbb{R}_0^4 \rightarrow \mathbb{R}_0^3$ with structure group $U(1)$. The compactness of the fiber will be a useful feature when we will discuss the quantum setting; moreover the very structure of a fibration allows an easy “dualization” of the case at hand. Infact, being π_{KS} a submersion, we can embed injectively $\mathcal{F}(\mathbb{R}_0^3)$ into $\mathcal{F}(\mathbb{R}_0^4)$ by

$$\pi_{KS}^* : f \in \mathcal{F}(\mathbb{R}_0^3) \rightarrow f \circ \pi_{KS} \in \mathcal{F}(\mathbb{R}_0^4) \quad (2.15)$$

In particular, the above map realizes $\mathcal{F}(\mathbb{R}_0^3)$ as the subalgebra of $\mathcal{F}(\mathbb{R}_0^4)$ made up by functions which are constant along the fibers.

In this algebraic context, we may now investigate the projectability of differential operators from \mathbb{R}_0^4 onto \mathbb{R}_0^3 and in particular of second order ones: at this aim, it will be very useful to characterize $\mathcal{F}(\mathbb{R}_0^3)$ using vector fields defined on \mathbb{R}_0^4 , in the following way.

From equation (2.12), one may observe that the orbits of the one parameter group $\exp(i\lambda\sigma_3)$ acting by right multiplication on $S^3 \times \mathbb{R}^+$ are the fibers of the KS-fibration. Hence, there is a natural action by automorphisms of $\exp(i\lambda\sigma_3)$ on $\mathcal{F}(\mathbb{R}_0^4)$ given by

$$(U_\lambda f)(g) = f(g \exp(i\lambda\sigma_3)) \quad (2.16)$$

with $g = Rs$, $s \in SU(2)$, $R \in \mathbb{R}^+$. Now, by equation (2.15), the elements f of $\mathcal{F}(\mathbb{R}_0^3)$ are the only ones which fulfill the condition

$$U_\lambda f = f \quad \forall \lambda \in \mathbb{R} \quad (2.17)$$

This condition can be expressed by saying that the infinitesimal generator \mathbf{X}_3 of U_λ annihilates *all and only* the functions constant along the fibers, i.e. $\text{Ker} \mathbf{X}_3 = \mathcal{F}(\mathbb{R}_0^3)$. Moreover, \mathbf{X}_3 is a left invariant vector field for the action of $SU(2)$, and in cartesian coordinates it has the expression

$$\mathbf{X}_3 = y^0 \frac{\partial}{\partial y^3} - y^3 \frac{\partial}{\partial y^0} + y^1 \frac{\partial}{\partial y^2} - y^2 \frac{\partial}{\partial y^1} \quad (2.18)$$

By means of the above vector field, we may give a condition for the projectability of differential operators of any degree. Let us consider the algebra \mathcal{C} generated by the monomials in \mathbf{X}_3 of any degree and $\mathcal{F}(\mathbb{R}_0^3)$ (i.e. a central Lie algebra extension of the enveloping algebra of \mathbf{X}_3). Projectable operators with respect to π_{KS} are then given by the *normalizer* of this extension in the algebra $\mathcal{D}(\mathbb{R}_0^4)$ of differential operators on $\mathcal{F}(\mathbb{R}_0^4)$, i.e. the set of elements D^N of $\mathcal{D}(\mathbb{R}_0^4)$ such that

$$[D^N, C] \in \mathcal{C}, \quad \forall C \in \mathcal{C} \quad (2.19)$$

One can easily show that if D^N satisfies the above equation, then it leaves invariant the subalgebra $\mathcal{F}(\mathbb{R}_0^3)$; indeed, one can prove that the commutator $[D, \mathbf{X}_3]$ is necessarily an *homogeneous* element of \mathcal{C} . It follows that

$$[D^N, \mathbf{X}_3](f) = 0 \quad \forall f \in \mathcal{F}(\mathbb{R}_0^3) \quad (2.20)$$

which implies

$$\mathbf{X}_3(D^N f) = 0 \quad \forall f \in \mathcal{F}(\mathbb{R}_0^3) \quad (2.21)$$

i.e. D^N leaves the subalgebra $\mathcal{F}(\mathbb{R}_0^3)$ invariant, that is it is projectable according to our definition (2.9).

The converse result is quite immediate, being aware of the fact that adding to a projectable differential operator an expression in \mathbf{X}_3 with arbitrary coefficients in $\mathcal{F}(\mathbb{R}_0^4)$ does not alter its projectability property.

The above characterization is general; however, for simplicity it is often useful to deal with the centralizer \mathcal{D}^C of \mathbf{X}_3 (instead of the normalizer of \mathcal{C}), i.e. the set of differential operators in $\mathcal{D}(\mathbb{R}_0^4)$ that commutes with \mathbf{X}_3

$$[\mathbf{D}^k, \mathbf{X}_3] = 0 \quad (2.22)$$

Differential operators in the centralizer are obviously projectable, since they satisfy eq. 2.19 in a trivial way. Although this is not a general condition, it will be very useful in our study, since one can show that, in the case at hand, the projections of all the elements in the centralizer of \mathbf{X}_3 cover all the differential operators in \mathbb{R}_0^3 . Because this property is sufficient for our future purposes, in the following we will deal only with differential operators in this centralizer; thus, we will characterize \mathcal{D}^C in some more detail.

The centralizer \mathcal{D}^C forms a subalgebra of $\mathcal{D}(\mathbb{R}_0^4)$; in particular it is a module over the subalgebra $\mathcal{F}(\mathbb{R}_0^3)$, not over the whole algebra because the point-wise product of a function which is *not* constant along the fibers with an element in $\mathcal{F}(\mathbb{R}_0^3)$ does not give again a function constant along the fibers. The interesting result is that this subalgebra \mathcal{D}^C may be constructed in the following way from a set of projectable fields and functions which are constant along the fibers. One starts by introducing a “basis” of $\chi(S^3 \times \mathbb{R}^+)$ set up by three basis vector fields on S^3 (as it is parallelizable) and a field on \mathbb{R}^+ , which commutes with all the others, because of the structure of Cartesian product.

One can choose a basis on S^3 given by the three right invariant vector field, $\mathbf{Y}_1, \mathbf{Y}_2, \mathbf{Y}_3$, that, from general theory of Lie groups, commute with \mathbf{X}_3 , since it is a left invariant vector field. Adding a vector field \mathbf{R} on \mathbb{R}^+ , we have a basis of $\chi(\mathbb{R}_0^4)$ formed by projectable vector fields.

Having in mind what stated in the previous section, the differential operators on $\mathcal{F}(\mathbb{R}_0^4)$ belong to the algebra generated by monomials in $\mathbf{Y}_1, \mathbf{Y}_2, \mathbf{Y}_3, \mathbf{R}$ and elements in $\mathcal{F}(\mathbb{R}_0^4)$. In particular, the above monomials are projectable linear maps, in that their commutator with \mathbf{X}_3 satisfy condition (2.22), as can easily be seen just using the Leibniz rule with respect to the composition.

Now, consider the associative algebra generated by monomials in the above basis fields and elements of $\mathcal{F}(\mathbb{R}_0^3)$. Because the relation

$$[fD, \mathbf{X}_3] = f[D, \mathbf{X}_3] - \mathbf{X}_3(f)D \quad (2.23)$$

is satisfied by an arbitrary function f and a linear map D , all the elements of the above algebra commute with \mathbf{X}_3 , i.e. belong to \mathcal{D}^C , and so are projectable.

By the converse, decomposing (uniquely) a differential operator D in the

projectable basis, if it belongs to \mathcal{D}^C condition (2.22) immediately implies that the “functional coefficients” of \mathbf{D} are annihilated by \mathbf{X}_3 .

So we have given a useful characterization of the centralizer of \mathbf{X}_3 as the elements generated by monomials in the above basis with “functional coefficient” belonging to $\mathcal{F}(\mathbb{R}_0^3)$. Using it we are able to show that the projections of the elements in \mathcal{D}^C actually cover the differential operators on \mathbb{R}_0^3 .

One can start from considerations about the submodule of the vector fields. Since, when a vector field is projectable, the push-forward of this vector field evaluated at each point defines again a vector field, which coincides with its projection, one has an operative way to obtain the projection of a vector field. In this way one easily find that the push-forward of the vector fields of the basis $(\mathbf{R}, \mathbf{Y}_1, \mathbf{Y}_2, \mathbf{Y}_3)$ of $\chi(\mathbb{R}_0^4)$ with respect to the KS map are respectively a vector field along r and the generators of the three rotation of \mathbb{R}_0^3 .

Thus, the module M generated by the above basis, over the algebra $\mathcal{F}(\mathbb{R}_0^3)$ projects onto the module of the vector fields on \mathbb{R}_0^3 over the algebra $\mathcal{F}(\mathbb{R}_0^3)$: in fact, a basis of the first projects onto a system of generators of the second, and the map is $\mathcal{F}(\mathbb{R}_0^3)$ -linear, the underlying algebra being the same.

Using the fact that monomials in the elements of a system of generators (resp. a basis) of the Lie algebra of the vector fields on \mathcal{M} provide a systems of generator (resp. a basis) for the corresponding enveloping algebra, one can also show that the module of differential operators on \mathbb{R}_0^4 over the algebra $\mathcal{F}(\mathbb{R}_0^3)$ projects onto the module of differential operators on \mathbb{R}_0^3 .

3 Reduction and unfolding: quantum aspects

In this section we will use the tools introduced so far to study the problem of reduction of dynamical systems in quantum mechanics: actually, we will be concerned with the inverse procedure, the unfolding, which is highly not unique. However, we will focus on the quantum Kepler problem, i.e. the hydrogen atom, having in mind to clarify how an unfolding procedure may be defined for a quantum system. We leave aside the general treatment for a future study.

The link with the previous section relies on the fact that a quantum dynamical system with Hamiltonian operator \hat{H} is supposed to evolve in time accordingly to the Schrödinger equation

$$i\hbar\dot{\psi}(t) = \hat{H}\psi(t) \quad (3.1)$$

where ψ is a vector in a “functional” Hilbert space $\mathcal{H}_{\mathcal{N}}$ constructed over a “configuration manifold” \mathcal{N} . Generally, \hat{H} is represented on $\mathcal{H}_{\mathcal{N}}$ in terms of a (non homogeneous) differential operator of second degree: hence, it is natural to define an unfolding procedure for a quantum system in the following way. First of all, one searches for a higher dimensional configuration mani-

fold \mathcal{M} with a submersion $\pi : \mathcal{M} \rightarrow \mathcal{N}$, and a differential operator \hat{H}' which projects onto \hat{H} with respect to π . Then, one constructs an Hilbert space $\mathcal{H}_{\mathcal{M}}$ of “wave functions” which contains $\mathcal{H}_{\mathcal{N}}$ as a subspace, and on which the operator \hat{H}' extends the operator \hat{H} . As stated above, all the steps in this procedure are not unique. However, one may restrict the arbitrariness by the means of physical motivations, e.g. by introducing symmetries, etc: this is just what happens in our case of study.

Let us consider the following differential operator

$$\hat{H} = -\frac{\Delta_3}{2} - \frac{k}{r} \quad (3.2)$$

where Δ_3 is the Laplacian operator on \mathbb{R}_0^3 associated with the Euclidean metric, r is the radial coordinate, $k > 0$ is a coupling constant, and the Hilbert space $\mathcal{H}_{\mathbb{R}_0^3}$ is $\mathcal{L}^2(\mathbb{R}_0^3, d^3x)$. It is well known that \hat{H} describes the hydrogen atom in the center of mass system, where we have set $m = \hbar = 1$, and is the quantum analogue of the Kepler problem. It seems thus natural to us to relate the hydrogen atom with a differential (inhomogeneous) operator on \mathbb{R}_0^4 projectable with respect to the KS-fibration, as it happens in the classical counterpart. So, we search for a second order non-homogeneous differential operator \hat{H}' on \mathbb{R}_0^4 which projects onto \hat{H} ; since the multiplicative operator $k\hat{R}^{-2}$ obviously project on $k\hat{r}^{-1}$ (since $\pi_{KS}^*(r^{-1}) = R^{-2}$), we are left with the search for a second order differential operator D that projects on the Laplacian Δ_3 . It is obvious that there may be many such operators; however, we may drastically reduce this arbitrariness by symmetry requirements. Indeed, one knows that the algebra of invariance of the hydrogen atom in three dimensions is $\mathfrak{so}(4) \approx \mathfrak{su}(2) \times \mathfrak{su}(2)$, generated by the angular momentum and the Runge-Lenz vector ([16],[17]). It seems therefore reasonable to ask that the unfolding quantum system in 4 dimensions, and so D , shares the same symmetry property, so that $\mathfrak{su}(2) \oplus \mathfrak{su}(2)$ is at least a subalgebra of its algebra of invariance.

This request of invariance can be stated in term of invariance with respect to the algebra $\mathfrak{su}(2) \oplus \mathfrak{su}(2)$ generated by the direct product of the left action and the right action of $SU(2)$ that one naturally has on $S^3 \approx SU(2)$. To exploit this requirement, it is useful to decompose the problem in a spherical and a radial part (e.g. using the basis introduced in section 2.1). The radial part is obviously invariant under this action, so we only have to impose that the part on S^3 is invariant under left and right action of $SU(2)$. One knows ([18]) that the only second order differential operator with the above property is Δ_3^S , the Laplacian associated with S^3 . This excludes mixed terms (composition of operators along S^3 with the one along \mathbb{R}), implying that D must be of the form

$$D = f(R)\frac{\partial^2}{\partial R^2} + g(R)\frac{\partial}{\partial R} + h(R)\Delta_3^S + c(R) \quad (3.3)$$

where R is the radial coordinate in \mathbb{R}_0^4 .

Before imposing that D project on Δ_3 , we recall that Δ_3 can be expressed as

$$\Delta_3 = \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \Delta_2^S \quad (3.4)$$

where Δ_2^S is the Laplacian associated with S^2 .

Moreover, it can be easily proven that Δ_3^S does project onto Δ_2^S with respect to the Hopf fibration.

So, the requirement that the differential operator D as in eq. 3.3 projects onto Δ_3 as in eq. (3.4) with respect to the KS-fibration becomes just a conditions on the functions f, g, h, c , that in this way are fixed.

In the end, one finds that the differential operator that projects on Δ_3 , with the additional condition of invariance under $\mathfrak{su}(2) \oplus \mathfrak{su}(2)$ is:

$$D = \frac{1}{4R^2} \frac{\partial^2}{\partial R^2} + \frac{1}{2R^3} \frac{\partial}{\partial R} + \frac{1}{4R^4} \Delta_3^S = \frac{1}{4R^2} \Delta_4 \quad (3.5)$$

where Δ_4 is the Laplacian operator associated with the Euclidean metric.

It follows that \hat{H}' is expressed as

$$\hat{H}' = -\frac{1}{2} \frac{1}{4R^2} \Delta_4 - \frac{k}{R^2} \quad (3.6)$$

Usually, the operator \hat{H}' is referred to as the *conformal Kepler* Hamiltonian. The last step in this unfolding procedure involves the construction of a Hilbert space $\mathcal{H}_{\mathbb{R}_0^4}$ of functions over \mathbb{R}_0^4 on which \hat{H}' is defined. At first sight one may think to choose $\mathcal{L}^2(\mathbb{R}_0^4, d^4y)$ with d^4y the Lebesgue measure on \mathbb{R}^4 : however, the operator \hat{H}' is by no means symmetric on this Hilbert space. Hence, we may search for a measure on \mathbb{R}_0^4 which induces a scalar product on $\mathcal{F}(\mathbb{R}_0^4)$ so that \hat{H}' is symmetrically defined. Actually, the operator \hat{H}' should be (essentially) selfadjoint on its domain in order to assure the existence of a unitary dynamics, i.e. a one parameter group of a unitary time evolution: however, we leave for a later section the analysis of this question, in which we will also argue that “the search for a selfadjoint Hamiltonian” is an echo of the reparametrization of the dynamical field which happens in the classical case.

Let us consider the Hilbert space $\mathcal{H}_{\mathbb{R}_0^4} = \mathcal{L}^2(\mathbb{R}_0^4, 4R^2 d^4y)$: if one chooses the set of C^∞ functions with compact support

$$\mathcal{D} \equiv C_0^\infty(\mathbb{R}_0^4) \quad (3.7)$$

which clearly belongs to $\mathcal{H}_{\mathbb{R}_0^4}$, the operator \hat{H}' becomes Hermitian on \mathcal{D} . Moreover, \mathcal{D} is dense in $\mathcal{H}_{\mathbb{R}_0^4}$, as one can prove by using the unitary operator

$$U : \mathcal{L}^2(\mathbb{R}_0^4, 4R^2 d^4y) \rightarrow \mathcal{L}^2(\mathbb{R}_0^4, d^4y) : \varphi \rightarrow 2R\varphi \quad (3.8)$$

which leaves the set \mathcal{D} invariant. Then, \hat{H}' is symmetric on \mathcal{D} : actually, one can prove that \hat{H}' is essentially selfadjoint on \mathcal{D} , by using the same arguments of [31] as in the proof of the essential self-adjointness of Laplacian operators in \mathbb{R}^n .

Now we will show that $\mathcal{H}_{\mathbb{R}_0^3}$ is contained as a subspace in $\mathcal{H}_{\mathbb{R}_0^4}$: this may be done easily using the following geometrical argumentation. The measure d^3x and $4R^2 dy_0$ are associated with two volume forms, which we denote by μ_3 and μ_4 respectively. Explicitly, in a Cartesian system of coordinate, one has

$$\begin{aligned}\mu_3 &= dx_1 \wedge dx_2 \wedge dx_3 \\ \mu_4 &= 4R^2 dy_0 \wedge dy_1 \wedge dy_2 \wedge dy_3\end{aligned}\tag{3.9}$$

Now, the following relation holds between μ_3 and μ_4

$$i_{\mathbf{X}_3}(\mu_4) = \pi_{KS}^*(\mu_3)\tag{3.10}$$

and then we may factorize μ_4 in the form

$$\mu_4 = \pi_{KS}^*(\mu_3) \wedge \Theta_3,\tag{3.11}$$

where Θ_3 is a dual field³ to \mathbf{X}_3 .

Now consider two functions \tilde{f}, \tilde{g} costant along the fibers: from the previous section we know that such functions are of the form $\tilde{f} = \pi_{KS}^*(f)$ and $\tilde{g} = \pi_{KS}^*(g)$, with f and g uniquely determined. Then, by using some general theorems ([25], [29]) about the integration of forms along fibers of the bundle space of a fibration, one has that

$$\begin{aligned}\int_{\mathbb{R}_0^4} \tilde{f} \tilde{g} \mu_4 &= \int_{\mathbb{R}_0^4} \tilde{f} \tilde{g} \pi_{KS}^*(\mu_3) \wedge \Theta_3 \\ &= \int_{\mathbb{R}_0^3} \bar{f} g \mu_3 \int_{U(1)} \Theta_3 \\ &= c \int_{\mathbb{R}_0^3} \bar{f} g \mu_3\end{aligned}\tag{3.12}$$

where c does not depend on the pair of functions \tilde{f} and \tilde{g} . To obtain the result above, we have mainly used that Θ_3 is dual to the tangent field to the fiber, and that the fiber itself is compact. So, we have been able to “integrate out” the fiber contribute, hence to show that the KS-map π_{KS}^* gives rise (up to a constant scaling factor) to an isometric embedding U_{KS} of $\mathcal{H}_{\mathbb{R}_0^3}$ into $\mathcal{H}_{\mathbb{R}_0^4}$.

³Any dual fields of form suits well for our purposes, and we may select one e.g. by requiring left invariance

3.1 Eigenvalue equation

At this point we may study the eigenvalue equation for \hat{H}' on $\mathcal{H}_{\mathbb{R}_0^4}$: obviously, because of our unfolding procedure, the set of solutions of this equation contains properly that of the eigenvalue problem of the hydrogen atom on $\mathcal{H}_{\mathbb{R}_0^3}$, and are precisely those solutions which are constant along the fibers. Then, we consider the following equation

$$\left(-\frac{1}{2}\frac{1}{4R^2}\Delta_4 - \frac{k}{R^2}\right)\psi - E\psi = 0 \quad (3.13)$$

which defines a subspace in $\mathcal{F}(\mathbb{R}_0^4)$.

This same subspace is also defined by the equation

$$\left(-\frac{1}{2}\Delta_4 - 4R^2E\right)\psi - 4k\psi = 0 \quad (3.14)$$

So, if we are interested in bound states of the hydrogen atom ($E_n < 0$), the equation (3.13) may be conveniently replaced by equation (3.14), which represents an eigenvalue equation for a “family of isotropic quantum harmonic oscillator” with frequency $\omega(E) = \sqrt{-8E}$ depending on the energy. We then find a “metamorphosis” ([32]) of the coupling constant k into an eigenvalue; we can determine the “admissible frequencies” by imposing that

$$4k = \omega(E)(N + 2), \quad N \in \mathbb{N} \quad (3.15)$$

and then

$$E_N = -\frac{2k^2}{(N + 2)^2} \quad (3.16)$$

As we stated above, not all the solutions of equation (3.14) are solutions of the eigenvalue problem for the three-dimensional hydrogen atom: infact, we have to select the projectable ones, i.e. the functions ψ which are constant along the fibers. So, we must impose

$$\mathbf{X}_3\psi_N = 0 \quad (3.17)$$

Recalling the expression (2.18), and using the knowledge of the solutions of equation (3.14) (products of Hermite functions), one finds that N should be an even natural number

$$N = 2m, \quad m \in \mathbb{N} \quad (3.18)$$

Then, the eigenvalues corresponding to the projectable eigenfunctions are

$$E_m = -\frac{k^2}{2(m + 1)^2}, \quad m \in \mathbb{N} \quad (3.19)$$

and one easily recognizes the energy level of the hydrogen atom, taking into account the fact that m starts from 0.

Thus, we have found the spectrum of the hydrogen atom and the corresponding eigenfunctions (with the correct multiplicity) by solving the unfolding system, which is related to a family of harmonic oscillators.

3.2 Reduction of symmetry

For the sake of completeness, in this section we briefly discuss how the symmetry algebra of the conformal Kepler problem in 4 dimensions reduces to the symmetry algebra of the Kepler problem in 3 dimensions. This topic has been the subject of extensive studies, and here we just want to present it in our perspective, i.e. in the setting of the projectability of differential operators on a manifold; we refer to the literature for details.

First of all, one has to characterize the symmetry algebra of the conformal Kepler problem. This can be done, and was done (see [33]), starting from the symmetry of the harmonic oscillator: one first restricts to each eigenspace, where the conformal Kepler problem is related to an harmonic oscillator, and then extends the algebra so obtained to (a suitable domain of) the whole Hilbert space (cfr. with the classical case, ref. [8]). It is well known that the symmetry algebra of an n -dimensional harmonic oscillator is $\mathfrak{u}(n)$, whose generators are, in terms of differential operators⁴ on \mathbb{R}_0^4

$$\hat{L}_{\alpha\beta} = y^\alpha \frac{\partial}{\partial y^\beta} - y^\beta \frac{\partial}{\partial y^\alpha} \quad (3.20)$$

$$\hat{D}_{\alpha\beta}^E = \frac{1}{2} \left(\omega^2(E) y^\alpha y^\beta + \frac{\partial^2}{\partial y^\alpha \partial y^\beta} \right) \quad (3.21)$$

There is an isomorphism between this algebra and the algebra of complex 4×4 anti-Hermitian matrices; each matrix C of this kind can be split in the sum of two real matrices as $C = A + iB$; $A = -A^T$, $B = B^T$: the $\hat{L}_{\alpha\beta}$ correspond to the antisymmetric ones, the $\hat{D}_{\alpha\beta}$ to the symmetric ones.

Thus, the operators above, when restricted to each eigenspace of \hat{H}' corresponding to the eigenvalue E , represent symmetries for \hat{H}' . They can be extended to the whole Hilbert space, with some care due to the fact that the resulting operators have to be (essentially) selfadjoint and to commute with \hat{H}' (on the intersection of their domains).

The $\hat{L}_{\alpha\beta}$ satisfy automatically these properties (being the generators of the rotations); so do also the $\hat{D}_{\alpha\beta}$, providing that one replace the value of the eigenvalue with the Hamiltonian (for a more careful explanation see [33]). So, the symmetry algebra of the conformal Kepler problem is $\mathfrak{u}(n)$, represented by:

$$\hat{L}_{\alpha\beta} = y^\alpha \frac{\partial}{\partial y^\beta} - y^\beta \frac{\partial}{\partial y^\alpha} \quad (3.22)$$

$$\hat{D}_{\alpha\beta} = \frac{1}{2} \left(-2y^\alpha y^\beta \hat{H}' + \frac{\partial^2}{\partial y^\alpha \partial y^\beta} \right) = \frac{1}{2} \left(\frac{y^\alpha y^\beta}{R^2} \Delta_4 + 2k \frac{y^\alpha y^\beta}{R^2} + \frac{\partial^2}{\partial y^\alpha \partial y^\beta} \right) \quad (3.23)$$

⁴Their expression in terms of the creation and annihilation operators is more familiar, but not suitable for their extension from each eigenspace to the whole Hilbert space

In our scheme, to obtain the symmetry algebra of the three dimensional Kepler problem, one has to consider the subalgebra of the whole symmetry algebra of the unfolding system made of projectable operators. Since, in our specific case, the centralizer of \mathbf{X}_3 covers the differential operators on \mathbb{R}_0^3 , we can restrict our analysis to the subalgebra of the symmetry algebra $\mathfrak{u}(4)$ of differential operators in this centralizer.

To obtain the combinations of $\hat{L}_{\alpha\beta}$ and $\hat{D}_{\alpha\beta}$ that commute with \mathbf{X}_3 , it is easier to first restrict to each eigenspace of \hat{H}' , where we can use the isomorphism with the algebra of matrices, as above. The problem is then to find those matrices, among the symmetric and antisymmetric ones, that commute with the matrix representative of \mathbf{X}_3 : this problem is exactly the same as in the classical case, and has already been solved in that setting (see [8], [34]). We will not do it again here, but give the result in terms of differential operators.

As for the antisymmetric ones, we are left with the three operators \hat{L}_i , i.e. the three right invariant vector fields on the 3-sphere

$$\begin{aligned}\hat{L}_1 &:= \hat{L}_{10} + \hat{L}_{32} = \mathbf{Y}_1 \\ \hat{L}_2 &:= \hat{L}_{02} + \hat{L}_{13} = \mathbf{Y}_2 \\ \hat{L}_3 &:= \hat{L}_{03} + \hat{L}_{21} = \mathbf{Y}_3\end{aligned}\tag{3.24}$$

As for the $\hat{D}_{\alpha\beta}$, one obtains the following combinations:

$$\hat{D}_1 = \frac{1}{2} \left\{ (y^1 y^3 + y^2 y^0) (-2E) E + \frac{\partial^2}{\partial y^1 \partial y^3} + \frac{\partial^2}{\partial y^2 \partial y^0} \right\} \tag{3.25}$$

$$\hat{D}_2 = \frac{1}{2} \left\{ (y^2 y^3 - y^1 y^0) (-2E) + \frac{\partial^2}{\partial y^2 \partial y^3} - \frac{\partial^2}{\partial y^1 \partial y^0} \right\} \tag{3.26}$$

$$\hat{D}_3 = \frac{1}{4} \left\{ ((y^1)^2 + (y^2)^2 - (y^3)^2 - (y^0)^2) (-2E) + \right. \tag{3.27}$$

$$\left. + \frac{\partial^2}{\partial (y^1)^2} + \frac{\partial^3}{\partial (y^2)^2} - \frac{\partial^2}{\partial (y^3)^2} - \frac{\partial^2}{\partial (y^0)^2} \right\} \tag{3.28}$$

While the antisymmetric operators are well defined on the whole Hilbert space, for the symmetric one we replace E with the Hamiltonian operator, as explained above. In the end, we have a set of 6 differential operators that commute with \mathbf{X}_3 and satisfy the following commutation relations:

$$\begin{aligned}[\hat{L}_i, \hat{L}_j] &= i\epsilon_{ijk} \hat{L}_k \\ [\hat{L}_i, \hat{D}_j] &= i\epsilon_{ijk} \hat{D}_k \\ [\hat{D}_i, \hat{D}_j] &= i\epsilon_{ijk} \hat{L}_k (-2\hat{H}')\end{aligned}\tag{3.29}$$

i.e. they close an $\mathfrak{so}(4)$ algebra⁵, as happened in the classical case.

Now it is quite easy to find the explicit expressions of the projections of the above operators on $\mathcal{L}^2(\mathbb{R}^3, d^3x)$, following the method suggested in the first section. As for the \hat{L}_i , they are the three right invariant vector fields on the 3-sphere, and we have already pointed out (at the end of section 2.1) that they project on the three generators of the rotation in \mathbb{R}_0^3 , so on the angular momentum operators on $\mathcal{L}^2(\mathbb{R}^3, d^3x)$.

One can also explicitly find the projections of the \hat{D}_i , using that \hat{H}' projects on \hat{H}' , the monomials in the y^α on the x^i and that

$$\frac{\widetilde{\partial^2}}{\partial y^\alpha \partial y^\beta} = \frac{\partial^2 x^i}{\partial y^\alpha \partial y^\beta} \frac{\partial}{\partial x^i} + \frac{\partial x^i}{\partial y^\alpha} \frac{\partial x^j}{\partial y^\beta} \frac{\partial^2}{\partial x^i \partial x^j} \quad (3.30)$$

Putting all this together, one finds that the \hat{D}_i project on the components of the Runge-Lenz vector on $\mathcal{L}^2(\mathbb{R}^3, d^3x)$.

Summarizing, we have found the subalgebra of the whole symmetry algebra of the unfolding system of projectable operators, and found the explicit form of the projected operators on $\mathcal{L}^2(\mathbb{R}^3, d^3x)$, without the need to refer to a special coordinate system (as in previous works); the resulting algebra is $\mathfrak{so}(4)$ and the projected operators are the angular momentum and the Runge-Lenz vector, as we expected.

4 Reparametrization in the quantum realm: a proposal

In the previous section we have established the relationship between the three-dimensional hydrogen atom and a family of harmonic oscillators, in the sense that we have linked *each* eigenvalue equation for the hydrogen atom with *an* eigenvalue equation for an isotropic harmonic oscillator with frequency $\omega(E) = \sqrt{-8E}$ depending on the energy, where the eigenvalue is fixed and equal to the coupling constant k . This is exactly what happens in the classical case (see [8]): the unfolding of the Kepler problem in three dimension is achieved via a conformal Kepler problem in 4 dimension, that is related to a family of harmonic oscillators with frequency depending on the energy of the Kepler problem. We notice that in the classical case a reparametrization was involved; thus, to complete the parallelism, we expect that some kind of reparametrization is involved also in the quantum case. This section is devoted to this aim, and before doing that we need a clarification of *what is* reparametrization in the quantum realm, since this notion itself is not obviously clear.

First of all, we remark that reparametrization, in the classical setting, is

⁵Obviously, one can rescale by an appropriate function of the Hamiltonian, taking into account that we are restricting to the negative part of its spectrum.

connected with two different aspects, that is worthwhile to clarify separately, in order to better understand how one can think of it within the quantum setting.

The first aspect, the most immediate one, is that the reparametrization of a vector field preserves its integral curves: a vector field \mathbf{X} and any reparametrization $\tilde{\mathbf{X}} = f \cdot \mathbf{X}$ have the same integral curves, but with different parametrizations. In an intuitive way, when $f = a$ constant, the tangent vector to each integral curve at each point is dilated by a constant factor a , that corresponds to changing the parameter of the integral curves from t to $\tau = at$; this interpretation can be carried over also when f is a function on the manifold. In this sense, since the parameter of the integral curves of the dynamical vector field is interpreted as the “time”, reparametrization is connected to a “change of time”, i.e. one changes the way of measuring the time, dilating it by a factor f , either constant or depending on the point.

The other aspect of reparametrization is related to the completeness of vector fields. A vector field $\mathbf{X} \in \chi(\mathcal{M})$ is said to be *complete* when its flow defines an action of the group \mathbb{R} on \mathcal{M} (of which \mathbf{X} is the infinitesimal generator). A well known theorem assures that, given a non complete vector \mathbf{X} on a paracompact manifold \mathcal{M} , it is always possible to find a (strictly positive) function $f \in \mathcal{F}(\mathcal{M})$ such that $\tilde{\mathbf{X}} = f \cdot \mathbf{X}$ is complete. In other words, the reparametrization can be seen as a way to obtain a complete vector field out of one which is not complete.

Let us now examine what are the possible “quantum” counterparts of these two aspects. In fact, classically they are very closely related, being two different ways to see the same operation, i.e. the multiplication of a vector field by a function, while in the quantum setting things are not so straight. As for the first aspect, in the following consideration we restrict ourselves to maximally superintegrable system, i.e. n -dimensional systems with $2n - 1$ constants of the motion F_i ; we recall that the Kepler problem, as well as the harmonic oscillator, have this property. In this case (with the necessary regularity requirements), each integral curve of the dynamical vector field is uniquely determined by the values of these $2n - 1$ functions, i.e. by the intersection of the submanifolds $F_i = c_i$. In other words, the constants of the motion bear all the information about the motion, up to reparametrization. So, the search for a transformation on a vector field that leaves invariant its integral curves up to reparametrization is equivalent to the search for a transformation on a vector field that does not change its constants of the motion. Since the constants of the motion are solution of the equation

$$\mathbf{X}F_i = 0 \tag{4.1}$$

one can look for the transformations that leave it invariant.

It is evident that the multiplication for a function does not affect the solutions of the above equations: in this way one can recover the usual reparametrization of a vector field.

In the quantum setting, where we mainly deal with (partial) differential equation, the above line can serve as a guide (at least formally). Now the equations that encode the dynamical features of the system into account are the eigenvalue equations

$$(\hat{H} - E\mathbb{I})\psi = 0 \quad (4.2)$$

As above, one can look for the transformations on these equations that leave invariant the space of solutions (i.e. the eigenfunctions). There can be many of them. However, for analogy with the classical counterpart, let us restrict to the multiplication by a function⁶, that clearly has this property. One can look for those functions f such that

$$f(\hat{H} - E\mathbb{I})\psi = (\hat{H}'_E - \lambda_E\mathbb{I})\psi = 0 \quad (4.3)$$

i.e. such that the eigenvalue equation for \hat{H} (4.2) can be written as an eigenvalue equation for a different operator \hat{H}' , possibly depending on E . In that case we talk of reparametrization of the differential operator \hat{H} , and call the operator \hat{H}' that verifies eq. (4.3) the reparametrized operator.

A complete analysis of this proposal and of all its implication still has to be done and will be the subject of a subsequent paper. Here we only point out how the motivations for it come from the present case of study, i.e. the relationship between hydrogen atom and harmonic oscillator: what we have done at the end of the last section, eq. (3.13), (3.14) (that is what was usually done in previous papers in a somewhat hidden way) is exactly what we have tried to clarify here, putting it in a bit more general context.

As for the other aspect of reparametrization of a vector field, the one connected with its completion, we notice that there is a link between the completeness of a vector field and the self-adjointness of the corresponding (in a sense to be specified later) operator. This can be understood from a physical point of view by noticing that, when dealing with Hamiltonian vector fields that are not complete, the “quantization” of the corresponding Hamiltonian gives an Hamiltonian operator which is not self-adjoint (some explicit examples are presented in [35]). In other words, what happens is that, if the classical equation of the motion does not admit *global* solutions for arbitrary initial condition, i.e. trajectories defined for all $t \in (-\infty, +\infty)$, the corresponding quantum Hamiltonian will not be self-adjoint, unless one does not impose additional (and arbitrary) conditions (and this can even not be sufficient); this is what Klauder refers to as the “classical symptoms” of a quantum illness (the lack of self-adjointness).

This can be seen in more general and mathematically sophisticated terms, by the means of some results by Nelson ([36]) and a successive application by

⁶It is worthwhile to point out explicitly that this operation is meaningful since we are dealing with differential operators on a manifold, i.e. with a specific representation. In the abstract setting of operators it would make no sense to multiply by a function an abstract operator.

Hunziker ([37]; see also [38], p21-22 for a concise presentation).

All this appears in our case of study, as mentioned in the previous section. There we have dealt with the Hamiltonian \hat{H}' of the conformal Kepler problem which is not self-adjoint on the Hilbert space $\mathcal{L}^2(\mathbb{R}^3, d^4y)$ with d^4y the Lebesgue measure on \mathbb{R}^4 , and we have found a measure $d\mu$ with respect to which \hat{H}' is essentially self-adjoint (on a suitable domain); explicitly, we had $d\mu = 4R^2 d^4y$. This change of the measure has realized what we are referring to as the quantum analogue of the second aspect of reparametrization of a vector field: namely, while in the classical setting we multiplied the vector field by a function in order to make it complete, in the quantum setting we change⁷ the measure in order to make the Hamiltonian (essentially) self-adjoint.

In this sense the change of the measure is an echo of the reparametrization of the dynamical vector field. However, the whole problem needs further clarification, and we shall come back to some of the raised issues elsewhere.

5 Conclusions

The main aim of this paper is to contribute to the “geometrization” of quantum mechanics. In particular, we have presented some ideas to deal with reduction procedure in a systematic way. We have introduced an approach based on differential operators, in order to preserve the geometrical aspects of classical reduction procedure. We have considered as a case of study the hydrogen atom, guided by the classical treatment of the Kepler problem carried over in a previous work ([8]). Using our approach supplemented by symmetry requirements, we have arrived at a possible unfolding system and recovered the relationship with a family of harmonic oscillators, in analogy with the classical case.

Thanks to the systematic character of this procedure, we think that this procedure could be applied to other cases of physical interest; in particular, it would be interesting to work out this technique to quantum mechanical systems with continuous spectrum, in order to analyze, for example, the scattering states.

Moreover, there are still open issues about “quantum reparametrization”, which we hope to clarify elsewhere.

⁷In our specific case, the new measure $d\mu$ is the old Lebesgue measure multiplied by a function that is exactly the same that appears in the reparametrization of the classical vector field: it is not clear to us if this is a peculiarity of the present problem, or a general feature

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